Comment on ‘Effective polar potential in the central force Schrödinger equation’

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Abstract. We analyze a recent pedagogical proposal for an alternative treatment of the angular part of the Schrödinger equation with a central potential. We show that the authors' arguments are unclear, unconvincing and misleading.

In a recent paper Shikakhwa and Mustafa [1] put forward an alternative pedagogical discussion of the angular part of the solution to the Schrödinger equation for a quantum–mechanical model with a central force:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi \tag{1}$$

They devoted part of the paper to show that this equation is separable in spherical coordinates: $\psi(r,\theta,\phi) = R(r)\Theta(\theta)e^{im\phi}$, where $m = 0, \pm 1, \ldots$, a discussion that appears in almost every introductory textbook on quantum mechanics or quantum chemistry [2,3].

In particular, the authors concentrated on the polar equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d\Theta}{d\theta} - \frac{m^2}{\sin^2\theta} = -l(l+1)\Theta \tag{2}$$

where $l = 0, 1, \ldots$ is the angular–momentum quantum number. They proposed to convert this Sturm–Liouville equation into the Schrödinger–like one

$$-\frac{1}{2}\frac{d^2y(\theta)}{d\theta^2} + \frac{m^2 - \frac{1}{4}}{2\sin^2\theta}y(\theta) = Wy(\theta) \tag{3}$$

where $y(\theta) = \sin^{\frac{1}{2}}\theta\,\Theta(\theta)$ and $W = W_l = (1/2)[l(l+1) + 1/4]$. We want to call the reader's attention to the misleading notation used by the authors who called E to the eigenvalue of this equation as if it where the energy of the central–field model (1) (see their equations (12) and (14)). To avoid such misunderstanding we choose the symbol W for the eigenvalue of the polar equation. We think that for a pedagogical discussion it would have been more reasonable that the authors had chosen a rigid rotator in which case the eigenvalue of the polar equation is proportional to the energy of the system. It is worth adding that the transformation of a Sturm–Liouville problem like (2) into a Schrödinger equation like (3) is well–known since long ago.

If we rewrite $|m| = 0, 1, \ldots, l$ as $l = |m| + n$, $n = 0, 1, \ldots$ then we derive the correct form of the eigenvalue of the polar equation in terms of m and n

$$W_l = \frac{1}{2}\left(l + \frac{1}{2}\right)^2 = \frac{1}{2}\left(n + |m| + \frac{1}{2}\right)^2 \tag{4}$$

which shows that W_l does not depend on the sign of m, as expected from the fact that the effective polar potential in Eq. (3) depends on m^2. On the other hand, the authors' polar energy E_n^m (see their equation (14)) depends on m and does not clearly reflect the degeneracy just mentioned. In order to derive their expression the authors resorted to the following unconvincing and rather misleading argument "These solutions are for non–negative m; those for negative m are–as is well known–directly proportional to these solutions." The proportionality factor is in fact $e^{\pm i|m|\phi}$ and reflects part of the degeneracy of the central–field models; for that reason one should not neglect it so lightly.

The authors state that "The solutions $|P_l^m(\cos\theta)|^2$ represent the probability of finding the particle at a certain angle θ". They seemed to have forgotten the normalization factor N_l^m and that the polar part of the volume element is $\sin\theta\, d\theta$ because the actual probability for finding the particle between θ and $\theta + d\theta$ is well known to be $|N_l^m P_l^m(\cos\theta)|^2 \sin\theta$. Besides, $|P_l^m(\cos\theta)|^2$ is not a *solution* to the polar equation.

The eigenvalue W_l increases with $|m|$ as shown by Eq. (4). In order to explain this behaviour Shikakhwa and Mustafa [1] plotted the polar potential for increasing values of $|m|$ and showed that the minimum increases. We agree that this graphical procedure is illustrative, but the well–known Hellmann–Feynman theorem [2] is more elegant and rigorous, and should be added to the discussion. If we consider the eigenvalue equation $\hat{A}y = Wy$ ($y(0) = y(\pi) = 0$) for the operator

$$\hat{A} = -\frac{1}{2}\frac{d^2}{d\theta^2} + \frac{\lambda}{\sin^2\theta} \tag{5}$$

where λ is real, then that theorem states that

$$\frac{dW}{d\lambda} = \left\langle \sin^{-2}\theta \right\rangle > 0 \tag{6}$$

Clearly, as $|m|$ increases λ increases and W_l increases.

Summarizing, we think that the paper by Shikakhwa and Mustafa [1] is not suitable for pedagogical purposes for the following reasons: first, they apparently mistook the eigenvalue of the polar equation for the total energy of the central field model, second, the treatment of the polar equation (3) is unclear and misleading. In particular, the polar eigenvalue in their equation (14) does not clearly reveal the degeneracy coming from the sign of m, and the argument for the restriction to $m \geq 0$ in their expressions for the polar eigenvalue and eigenfunction is unconvincing and unnecessary. In fact, the correct result follows straightforwardly from the form of W_l as we have already shown above. Besides, the same simple argument clearly shows that $P_l^{|m|}(\cos\theta) = P_{|m|+n}^{|m|}(\cos\theta)$ which is consistent with the textbook treatment of the problem [2, 3]. We should also add the sloppy discussion of the probability of finding the particle in a given region of space.

[1] Shikakhwa M S and Mustafa M 2010 *Eur. J. Phys.* **31** 151.

[2] Cohen-Tannoudji C, Diu B, and Laloë F 1977 *Quantum Mechanics* (John Wiley & Sons, New York).

[3] Eyring H, Walter J, and Kimball G E 1944 *Quantum Chemistry* (John Wiley & Sons, New York).